RIOT portlet user guide

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In very general terms, to reduce a chemical reaction model, RIOT finds its smallest submodel that satisfies:

$$\left|F_T^{reduced\ model}(\boldsymbol{\phi}) - F_T^{full\ model}(\boldsymbol{\phi})\right| \leq abs.tol + rel.tol * \left|F_T^{full\ model}(\boldsymbol{\phi})\right| \quad (1)$$

$$\left|F_{species\ i}^{reduced\ model}(\boldsymbol{\phi}) - F_{species\ i}^{full\ model}(\boldsymbol{\phi})\right| \leq abs.tol + rel.tol * \left|F_{species\ i}^{full\ model}(\boldsymbol{\phi})\right| \quad (2)$$

where

$$F_T(\boldsymbol{\phi}) = \left.\frac{dT}{dt}\right|_{\boldsymbol{\phi}}, \quad (3)$$

$$F_{species\ i}(\boldsymbol{\phi}) = \left.\frac{dY_i}{dt}\right|_{\boldsymbol{\phi}}, \quad (4)$$

and

$$\begin{aligned} \boldsymbol{\phi} &\equiv (T, Y_1, Y_2, ..., Y_N) \quad (5)\\ T &\equiv Temperature \\ Y_i &\equiv mass\ fraction\ of\ species\ i \end{aligned}$$

Since these constraints are at single (discrete) points, valid range identification attempts to find a continuum (range) of temperatures and species concentrations over which the reduced model is known to satisfy the user-specified tolerances.

Choose Directory...

All files for the current RIOT job must be available in this directory. The comprehensive reaction mechanism must be provided as two chemkin-format files:

1. chem.inp (a text file describing the chemical elements, species and reactions that constitute the mechanism)
2. therm.dat (a text file of thermodynamic properties to be used with the mechanism)

See chemkin user manual for details on the formats of these files.

Other necessary RIOT files include premix.bin and/or oppdif.bin and/or save.dat (explained below).

Task

Reduce a model -

User's chemical reaction mechanism will be reduced, but valid range will not be found.

Reduce a model and find its Valid Range -

Both model reduction and valid range analysis will be performed.

NOTE: Model reduction is typically completed in a fractions of a second, while valid range analysis may require up to several minutes of CPU time. Note that valid range analysis is an iterative process in $N+1$ dimensions (where N=number of chemical species in model). Therefore, the computational expense of this process is strongly dependent on the initial guess (max. valid range) and the mechanism size.

Model Output

One Model per Point -

A reduced model will be obtained for each of the input points by applying constraints (1) and (2) at the corresponding point. Without further analysis, each reduced model is known to be valid at only one of the input points.

One Model -

One reduced model will be obtained for all of the input points by applying constraints (1) and (2) at all points simultaneously. Without further analysis, the resulting reduced model is known to be valid at all the input points.

Input Points

Values of $\boldsymbol{\phi}$ in equations (1) and (2). User can specify $\boldsymbol{\phi}$'s as grid points in chemkin premix or oppdif solution files (usually save.bin, but **must be renamed premix.bin or oppdif.bin respectively**), or as a text file ("save.dat") with pressure, temperature and species mass fractions (save.dat). The format for save.dat must be as follows:

$$
\begin{array}{l}
\text{Pressure} \\
\text{Temperature1 } Y_1\ Y_2\ \ldots\ldots\ldots\ldots\ldots\ldots\ Y_k \\
Y_{k+1}\ Y_{k+2}\ \ldots\ldots\ldots\ldots\ldots\ldots\ Y_N \\
\text{Temperature2 } Y_1\ Y_2\ \ldots\ldots\ldots\ldots\ldots\ldots\ Y_m \\
Y_{m+1}\ Y_{m+2}\ \ldots\ldots\ldots\ldots\ldots\ldots\ Y_N
\end{array}
\tag{6}
$$

etc. The first line in the file should contain only the pressure specified in units of dynes/cm^2 (1 dyne/cm^2 = 0.1Pascals). Temperature (units of Kelvin) and species mass frations should be space-delimited, with continuation permitted on subsequent lines. The number of values per line is unimportant (can use as little as one value per line or as many as desired), however specification of each new point must begin on a new line. **The order in which species mass fractions are specified must be the same for all points in a save.dat file, and must follow the order of species names in the chem.inp file (left to right across rows, with each line read in succession from top to bottom)**.

Model Reduction Tolerances

Temp. Absolute Tol -

Value of *abs.tol* in equation (1); units of Ks^{-1}.

Temp. Relative Tol -

Value of *rel.tol* in equation (1); dimensionless.

Species Absolute Tol -

Value of *abs.tol* in equation (2); units of s^{-1}.

Species Relative Tol -

Value of *rel.tol* in equation (2); dimensionless.

NOTE: *Global* tolerances are used for all species except those for which individual tolerances are specified.

Valid Range Identification

At the valid range identification level, equations (1) and (2) become:

$$\left|F_T^{reduced\ model}(\boldsymbol{\phi}) - F_T^{full\ model}(\boldsymbol{\phi})\right| \leq b_T * \left(abs.tol + rel.tol * \left|F_T^{full\ model}(\boldsymbol{\phi})\right|\right) \quad (7)$$

$$\left|F_{species\ i}^{reduced\ model}(\boldsymbol{\phi}) - F_{species\ i}^{full\ model}(\boldsymbol{\phi})\right| \leq b_S * \left(abs.tol + rel.tol * \left|F_{species\ i}^{full\ model}(\boldsymbol{\phi})\right|\right) \quad (8)$$

where b is an new parameter introduced to allow a definition of model validity different from that used for model reduction. If $b = 1$, the model will be considered valid only if it satisfies the model reduction tolerances. Changing the value of $b > 1$ allows the model to be valid at looser tolerances, (usually) leading to a larger valid range.

Temp. Error Tolerance buffers -

Value of b_T in equation (7); dimensionless.

Species Error Tolerance buffers -

Value of b_S in equation (8); dimensionless.

Max. Range -

RIOT searches for largest valid range by evaluating increasingly smaller ranges, beginning from the user-specified maximum. Therefore, identified valid range will be a sub-range of this user-specified max. range.i.e RIOT will search only within this range for the model valid range. ΔT and ΔC are defined in equations (9) and (10).

Min. Range -

RIOT will not search for valid range below this size. i.e quit search if max. valid range has been shrunk to this size and validity cannot be verified in this range. If any axes (T or C_i) exist with range sizes larger than the specified min. value for the axis, shrink range by shrinking these axes only, otherwise quit search with failure message.

$$\Delta T \equiv \frac{\bar{T} - T^{lowerbound}}{\bar{T}} = \frac{T^{upperbound} - \bar{T}}{\bar{T}} \tag{9}$$

$$\Delta C_i \equiv \frac{\bar{C}_i - C_i^{lowerbound}}{\bar{C}_i} = \frac{C_i^{upperbound} - \bar{C}_i}{\bar{C}_i} \tag{10}$$

Global values are used for all species except those for which individual values are specified.

NOTE: When a reduced model is generated using multiple points, the max. range is automatically set by RIOT using the minimum and maximum dimensions of the input points. For example, in a 2-species model, the input points:

1. T=350K, C_1=1.6e-5, C_2=8.5e-4
2. T=390K, C_1=2.5e-4, C_2=6.4e-4
3. T=325K, C_1=3.0e-4, C_2=1.5e-4

yield the max. range: T$\in$ [325, 390], $C_1\in$ [1.6e-5, 3.0e-4], $C_2\in$ [1.5e-4, 8.5e-4].

The min. range is set at $\Delta T = 1K$, and $\Delta C = 0.1$, using a nominal point as close to the center of the max. range as possible, maintaining the user-specified system pressure.